Supplementary Information

A Surface Site Interaction Model for the Properties of Liquids at Equilibrium

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Table S1. Experimental free energies of transfer measured at 298 K in kJ mol^{-1} (mole fraction standard state).

transfer of to from liquid	liquid liquid *n*-hexadecane	liquid liquid water	liquid liquid 1-octanol	liquid liquid diethyl ether	liquid *n*-hexadecane water	liquid 1-octanol water	*n*-octane *n*-octane liquid	water water liquid	ethanol ethanol liquid
n-pentane	-0.4	28.7	3.9		29.0	24.7		19.0	10.6
2-methylbutane		28.1			28.4			19.5	
n-hexane	-0.3	31.9	4.3		32.6	27.7	0.0	18.7	7.8
cyclohexane	-0.6	26.7	1.6		29.0	25.0	-0.3	20.5	9.6
n-heptane	-0.2	35.4	3.4		36.2	32.0		18.8	10.0
n-octane	-0.2	39.7	4.8	-0.1	40.0	35.0	0.2	18.4	9.7
2,2,4-trimethylpentane		36.7			36.8			19.7	
n-decane		49.8			46.9		0.2	18.5	8.1
n-dodecane		53.7						18.4	9.3
n-hexadecane							-0.2	18.1	8.8
water	18.0	0.0		6.0	-18.0	-3.2	39.8		3.2
methanol	10.2	1.0	0.1	2.9	-8.9	1.0			
ethanol	8.8	0.6	-3.0	1.4	-5.5	3.6	7.1	5.2	0.2
1-propanol	7.9	6.4	-0.4	1.9	-1.8	6.8	5.9		-0.3
2-propanol	7.6	7.5	1.8	1.9	-2.9	5.7	5.3		0.3
1-butanol	8.0	9.8	-0.6	1.6	2.0	10.4	5.1	1.6	-0.9
2-methyl-1-propanol	4.4	9.1						1.9	
2-butanol	6.8	8.4			0.9			0.7	
2-methyl-2-propanol	6.6			0.6	-0.6				
1-pentanol	7.5	13.4	-0.9	2.3	5.5	14.3		3.1	
3-methyl-1-butanol	9.0	12.9			5.6			2.7	
2-methyl-2-butanol	5.9	9.2			3.4			1.3	
1-hexanol	7.3	16.6	-0.4	1.9	9.1	17.0		2.9	
cyclohexanol	7.4	12.3	-0.1		5.5	12.4		2.1	
1-octanol	7.7	24.9	2.4	6.3	16.2	22.5	4.9	3.2	0.5
1-decanol	6.9	30.7	-0.8		23.8	31.5		3.5	
1-dodecanol		36.4	1.7			34.7		5.6	

2-methoxyethanol				2.9	-7.2		8.6		0.8
2-ethoxyethanol					-5.1				
ethylene glycol				10.1					
1,2-propanediol									
1,3-propanediol									
1,2-butanediol									
2R,3S-butanediol									
1,4-butanediol									
1,5-pentanediol									
diethylene glycol									
triethylene glycol									
diethyl ether	0.1	10.4	-0.1	0.2	11.8	10.5	-0.1	7.1	1.4
di-n-propyl ether	0.0	17.5	0.5		18.9	17.0		9.1	
diisopropyl ether	0.4	15.2	1.2		18.9	14.1	0.1	8.6	2.7
dibutyl ether	-0.3	25.0	1.2		25.8	23.8	0.3	10.7	3.9
1,2-dimethyoxyethane									
diethylene glycol dimethyl ether									
tetrahydrofuran	0.0	7.2	-0.9		7.4	8.1	1.5		1.4
2-methyltetrahydrofuran		8.5			9.2			3.6	
tetrahydropyran	-3.5	10.0	-0.8		11.3	10.8		5.0	

Table S2. Calculated free energies of transfer measured at 298 K in kJ mol^{-1} (mole fraction standard state).

transfer of to from liquid	liquid liquid *n*-hexadecane	liquid liquid water	liquid liquid 1-octanol	liquid liquid diethyl ether	liquid *n*-hexadecane water	liquid 1-octanol water	*n*-octane *n*-octane liquid	water water liquid	ethanol ethanol liquid
n-pentane	-0.3	26.7	0.3	-0.8	27.0	26.4	0.4	19.4	9.1
2-methylbutane	-0.4	26.7	0.3	-0.9	27.0	26.4	0.5	19.4	9.2
n-hexane	-0.3	30.5	0.4	-1.0	30.8	30.1	0.3	19.4	9.1
cyclohexane	0.0	27.0	0.6	-0.6	27.0	26.4	0.0	19.3	8.9
n-heptane	-0.4	34.3	0.4	-1.2	34.6	33.8	0.3	19.3	9.0
n-octane	-0.1	40.5	0.9	-0.9	40.5	39.6	0.0	19.3	8.9
2,2,4-trimethylpentane	-0.6	35.7	0.2	-1.7	36.3	35.5	0.5	19.3	9.0
n-decane	-0.2	48.0	1.0	-1.2	48.1	47.0	0.0	19.3	8.9
n-dodecane	-0.2	55.6	1.1	-1.5	55.7	54.4	0.0	19.3	8.9
n-hexadecane	0.0	73.7	1.8	-1.0	73.7	71.8	-0.1	19.2	9.0
water	19.2	0.0	6.4	3.0	-19.2	-6.4	40.5	0.0	3.3
methanol	9.6	0.2	2.0	2.3	-9.4	-1.8	2.1	0.8	-0.5

ethanol	9.0	3.3	1.5	1.6	-5.6	1.9	2.3	2.2	0.0
1-propanol	8.5	6.7	1.1	1.0	-1.9	5.6	2.1	3.2	0.3
2-propanol	8.4	6.6	1.0	0.9	-1.9	5.6	2.2	3.3	0.4
1-butanol	8.1	10.0	0.7	0.4	1.9	9.3	1.9	4.1	0.6
2-methyl-1-propanol	8.0	10.0	0.7	0.3	1.9	9.3	1.9	4.1	0.6
2-butanol	8.1	10.0	0.7	0.4	1.9	9.3	1.9	4.1	0.6
2-methyl-2-propanol	7.9	9.9	0.6	0.3	1.9	9.3	2.1	4.1	0.7
1-pentanol	7.7	13.4	0.4	-0.1	5.7	13.0	1.7	4.8	0.9
3-methyl-1-butanol	7.7	13.4	0.4	-0.2	5.7	13.0	1.7	4.8	0.9
2-methyl-2-butanol	7.6	11.2	0.2	-0.4	3.6	11.0	2.5	4.6	1.0
1-hexanol	7.4	16.9	0.2	-0.6	9.5	16.7	1.5	5.4	1.1
cyclohexanol	7.9	13.7	0.6	0.1	5.7	13.0	1.4	4.7	0.7
1-octanol	7.0	26.2	0.0	-1.1	19.2	26.2	0.9	6.4	1.5
1-decanol	6.5	33.4	-0.3	-1.9	26.8	33.6	0.8	7.2	1.8
1-dodecanol	6.1	40.5	-0.6	-2.6	34.4	41.1	0.7	7.8	2.1
2-methoxyethanol	10.7	-5.9	0.3	3.3	-16.6	-6.2	-0.1	-0.5	-0.6
2-ethoxyethanol	10.3	-2.4	0.1	2.8	-12.8	-2.5	0.5	0.4	-0.2
ethylene glycol	21.3	-5.7	5.8	6.6	-26.9	-11.5	4.7	-0.9	-0.5
1,2-propanediol	20.3	-2.9	4.9	5.4	-23.2	-7.8	4.5	0.2	-0.3
1,3-propanediol	20.4	-2.8	5.0	5.5	-23.2	-7.8	4.4	0.2	-0.3
1,2-butanediol	19.5	0.1	4.2	4.5	-19.4	-4.1	4.0	1.0	-0.2
2R,3S-butanediol	19.4	-1.9	4.0	4.5	-21.3	-5.9	4.7	0.9	0.1
1,4-butanediol	19.5	0.2	4.2	4.6	-19.4	-4.1	4.0	1.0	-0.2
1,5-pentanediol	18.8	3.3	3.6	3.7	-15.6	-0.3	3.5	1.7	-0.1
diethylene glycol	21.3	-12.6	3.2	6.7	-33.8	-15.7	0.9	-1.2	-0.9
triethylene glycol	21.6	-17.2	0.8	7.0	-38.8	-18.1	-0.7	-1.2	-1.0
diethyl ether	0.2	8.8	-2.1	0.0	8.5	10.8	-0.9	3.0	1.6
di-n-propyl ether	0.5	18.7	-1.6	0.1	18.3	20.3	-0.9	4.5	2.2
diisopropyl ether	0.1	16.2	-2.0	-0.4	16.1	18.3	-0.2	4.4	2.3
dibutyl ether	0.5	26.3	-1.4	-0.1	25.8	27.7	-0.6	5.4	2.7
1,2-dimethyoxyethane	0.8	-5.4	-4.4	0.7	-6.2	-1.0	-2.6	-0.1	-0.3
diethylene glycol dimethyl ether	1.3	-9.9	-6.5	1.2	-11.2	-3.3	-3.1	-0.5	-0.6
tetrahydrofuran	0.4	5.2	-2.0	0.3	4.7	7.1	-1.8	2.0	0.9
2-methyltetrahydrofuran	0.4	8.9	-1.9	0.2	8.5	10.8	-1.1	3.0	1.5
tetrahydropyran	0.5	9.0	-1.8	0.3	8.5	10.8	-1.3	2.9	1.4

Table S3. Association constants for formation of 1:1 complexes between DH and A in the gas phase at 298 K (M^{-1}).

DH	A	expt	calc
water	water	0.08	0.31
methanol	methanol	0.20	0.53
methanol	trimethylamine	1.28	1.57
ethanol	ethanol	0.40	0.55
Propan-2-ol	Propan-2-ol	0.60	0.66
t-Butyl alcohol	t-Butyl alcohol	0.79	0.75
pyrrole	trimethylamine	1.46	1.78
2,2,2-Trifluoroethanol	propionaldehyde	1.32	1.08
2,2,2-Trifluoroethanol	methanol	1.38	1.23
2,2,2-Trifluoroethanol	diethyl ether	1.58	1.50
2,2,2-Trifluoroethanol	acetone	1.72	1.84
2,2,2-Trifluoroethanol	tetrahydrofuran	1.91	1.90
2,2,2-Trifluoroethanol	ammonia	1.75	2.50
2,2,2-Trifluoroethanol	pyridine	2.28	2.64
2,2,2-Trifluoroethanol	trimethylamine	2.60	2.57
2,2,2-Trifluoroethanol	triethylamine	2.46	2.97
2,2,2-Trifluoroethanol	(Me2N)2C=NH	3.58	4.62
Hexafluoropropan-2-ol	methanol	1.93	1.95
Hexafluoropropan-2-ol	diethyl ether	2.26	2.28
Hexafluoropropan-2-ol	acetone	2.40	2.69
Hexafluoropropan-2-ol	tetrahydrofuran	2.75	2.77
Hexafluoropropan-2-ol	ammonia	2.76	3.51
Hexafluoropropan-2-ol	trimethylamine	3.91	3.59
Hexafluoropropan-2-ol	triethylamine	3.58	4.08
2,2,2-Trifluoro-1,1-bis(trifluoromethyl)ethanol	dimethyl ether	2.69	2.47
2,2,2-Trifluoro-1,1-bis(trifluoromethyl)ethanol	diethyl ether	2.83	2.63
2,2,2-Trifluoro-1,1-bis(trifluoromethyl)ethanol	acetone	3.04	3.07
2,2,2-Trifluoro-1,1-bis(trifluoromethyl)ethanol	tetrahydrofuran	3.58	3.16
2,2,2-Trifluoro-1,1-bis(trifluoromethyl)ethanol	ammonia	3.71	3.96
2,2,2-Trifluoro-1,1-bis(trifluoromethyl)ethanol	trimethylamine	5.20	4.05
2,2,2-Trifluoro-1,1-bis(trifluoromethyl)ethanol	triethylamine	4.53	4.58

Table S4. Association constants for formation of 1:1 complexes between DH and A in cyclohexane at 298 K (M^{-1}).

DH	**A**	expt	calc
pyrrole	tetrahydrofuran	-0.40	0.55
2-Chloroethanol	cyclopentanone	1.38	0.30
4-fluorophenol	c-propylamine	1.18	2.14
t-Butyl sulphide	pyridine N-oxide	-0.13	-0.73
N-methylaniline	N,N-dimethylacetamide	0.90	0.26
pyrrole	diethyl ether	-0.30	0.26
2,2,2-trichloroethanol	cyclopentanone	1.78	0.89
Isopropyl sulphide	pyridine N-oxide	-0.19	-0.73
diphenylamine	tetrahydrofuran	-0.40	0.20
diphenylamine	diethyl ether	-0.55	-0.05
carbazole	tetrahydrofuran	0.18	0.82
N-methylaniline	tributyl phosphate	0.86	0.39
phenol	tetrahydrothiophene	0.93	-0.21
4-chlorophenol	triethylamine	3.19	2.74
4-chlorophenol	isopropylamine	3.38	3.07
pyrrole	EtCN	1.04	0.21
4-chlorophenol	tetrahydrothiophene	1.00	-0.03
4-chlorophenol	1,4-dioxane	1.75	0.98
hexafluoropropan-2-ol	tetrahydrothiophene	1.17	0.22
4-chlorophenol	n-butylamine	3.31	3.05
chloroform	tributylamine	-0.55	-0.04
pyrrole	triethylamine	0.64	1.29
chloroform	triethylamine	-0.37	0.20
4-nitrophenol	diethyl ether	1.40	1.81
1-naphthol	benzene	-0.80	-0.98
N-methylaniline	Ph2CO	0.15	-0.59
pyrrole	1,4-dioxane	-0.10	0.06
Dichloromethane	pyridine N-oxide	0.38	0.22
4-fluorophenol	3-bromopyridine	1.11	1.45
chloroform	tributyl phosphate	0.72	0.54
chloroform	triethyl phosphate	0.75	0.61
aniline	N,N-dimethylacetamide	1.00	0.79
chloroform	HMPA	1.11	1.25
4-chlorophenol	morpholine	2.72	2.53
4-t-butylphenol	tetrahydrothiophene	0.53	-0.29
N-methylaniline	benzophenone	0.04	-0.60
4-chlorophenol	tripropylamine	2.42	2.15
N-methylaniline	acetone	0.08	-0.47
chloroform	dibutyl ether	-0.62	-0.64
N-methylaniline	ethyl acetate	-0.02	-0.64
diphenylamine	1,4-dioxane	-0.24	-0.23
4-fluorophenol	triethylamine	1.99	2.52
aniline	anisole	-0.14	-1.03
N-methylaniline	cyclohexyldimethylamine	-0.25	0.17
Chloroform	pyridine N-oxide	0.67	0.66
N-methylaniline	cyclohexanone	0.08	-0.39
2,2,2-Trichloroethanol	pyridine N-oxide	2.52	2.60
1-naphthol	toluene	-0.62	-0.98
aniline	tributyl phosphate	0.99	0.89
chloroform	quinuclidine	0.08	0.65
pyrrole	pyridine	0.74	1.04
3-trifluoromethylphenol	tetrahydrothiophene	0.78	0.10
4-fluorophenol	dimethyl sulphoxide	2.56	3.22
aniline	dipropyl ether	-0.30	-0.31
2,2,2-Trifluoroethanol	pyridine N-oxide	2.90	3.04
4-chlorophenol	tributylamine	2.39	2.25

4-fluorophenol	pyridine N-oxide	3.27	3.44
4-chlorophenol	tetrahydrofuran	1.41	1.63
3-methylphenol	1,4-dioxane	1.08	0.64
chloroform	1-methyl-2-pyrrolidone	0.51	0.47
aniline	ethyl acetate	0.20	-0.30
4-chlorophenol	triethylamine	2.29	2.74
4-t-butylphenol	N,N-dimethylacetamide	2.44	2.50
4-chlorophenol	diethyl ether	1.15	1.21
phenol	triethylamine	1.93	2.34
3-nitrophenol	diethyl ether	2.05	1.66
4-fluorophenol	1,4-dioxane	0.83	0.84
chloroform	c-hexylamine	0.04	0.40
N-methylaniline	anisole	-0.44	-1.24
Propan-1-ol	pyridine N-oxide	1.29	1.39
PhCCH	pyridine N-oxide	0.09	0.16
4-nitrophenol	triethylamine	3.10	3.58
N-methylaniline	pyridine	0.12	-0.09
1-naphthol	4-methylpyridine	1.96	2.32
chloroform	2,6-dimethylpyridine	-0.10	0.09
1-naphthol	p-xylene	-0.32	-0.73
3-fluorophenol	ethyl acetate	1.53	1.20
N-methylaniline	dipropyl ether	-0.51	-0.65
phenol	pyridine N-oxide	2.98	3.22
1-naphthol	1,4-dioxane	1.11	0.76
4-chlorophenol	triethylamine	2.35	2.74
4-nitro-3-trifluoromethylphenol	triethylamine	3.79	4.29
Pentafluorophenol	pyridine N-oxide	3.69	4.31
4-t-butylphenol	tetrahydrofuran	1.40	1.15
Hexafluoropropan-2-ol	pyridine N-oxide	3.73	4.35
N-methylaniline	N,N-dimethylaniline	-0.34	-0.95
2-naphthol	1,4-dioxane	1.11	0.78
1-naphthol	pyridine	1.83	2.09
aniline	benzene	-0.57	-1.50
4-fluorophenol	HMPA	3.80	4.68
3-fluorophenol	pyridine	2.42	2.44
3,4-dichlorophenol	triethylamine	2.75	3.14
chloroform	pentan-3-one	-0.14	-0.57
N-methylaniline	tetrahydrofuran	-0.11	-0.43
4-cyanophenol	triethylamine	2.97	3.38
1-naphthol	tetrahydrofuran	1.30	1.37
t-Butyl alcohol	pyridine N-oxide	1.26	1.42
carbazole	1,4-dioxane	0.40	0.28
chloroform	diethyl sulphide	-0.66	-1.10
4-t-butylphenol	pyridine	1.86	1.83
aniline	pyridine	0.23	0.37
chloroform	tetrahydrofuran	-0.27	-0.33
chloroform	cyclohexanone	0.00	-0.29
2-naphthol	diethyl ether	1.04	0.98
pyrrole	tetrahydropyran	0.68	0.39
Propan-2-ol	pyridine N-oxide	1.27	1.45
3-trifluoromethylphenol	ethyl acetate	1.63	1.38
1-naphthol	m-xylene	-0.28	-0.75
3-trifluoromethylphenol	pyridine	2.60	2.67
1-naphthol	diethyl ether	1.04	0.97
2-naphthol	tetrahydrofuran	1.34	1.38
pyrrole	1,4-dioxane	0.23	0.06
3-trifluoromethylphenol	cyclohexanone	1.85	1.95
3-fluorophenol	diethyl sulphide	0.41	0.13
aniline	N,N-dimethylaniline	-0.15	-0.67
chloroform	pyridine	0.15	0.03

chloroform	aniline	-0.29	-0.78
4-Chlorophenol	pyridine N-oxide	3.35	3.70
chloroform	ethyl acetate	-0.17	-0.55
chloroform	1,4-dioxane	-0.24	-0.68
4-t-butylphenol	triethylamine	2.03	2.13
1-naphthol	o-xylene	-0.30	-0.84
1-naphthol	3-methylpyridine	1.90	2.09
3,5-dichlorophenol	triethylamine	2.96	3.31
3-nitrophenol	triethylamine	3.02	3.37
Ethanol	pyridine N-oxide	1.28	1.50
4-chlorophenol	pyridine	2.32	2.41
3-trifluoromethylphenol	diethyl sulphide	0.69	0.25
4-chlorophenol	1,4-dioxane	1.20	0.98
1-naphthol	2-methylpyridine	1.94	2.12
dichloromethane	HMPA	0.15	0.69
pyrrole	pyridine N-oxide	1.61	1.99
phenol	dibutyl ether	0.93	0.78
aniline	Ph2CO	-0.05	-0.25
N-methylaniline	benzene	-0.85	-1.63
phenol	diethyl sulphide	0.30	-0.07
4-fluorophenol	pyridine	2.03	2.20
aniline	tetrahydrofuran	0.08	-0.05
4-fluorophenol	N,N-dimethylformamide	2.30	2.48
4-fluorophenol	benzonitrile	1.00	0.83
1-naphthol	mesitylene	-0.01	-0.59
3-methylphenol	diethyl ether	1.00	0.89
chloroform	tetrahydrothiophene	-0.55	-1.17
chloroform	acetone	-0.17	-0.37
3-methylphenol	tetrahydrofuran	1.28	1.21
Methanol	pyridine N-oxide	1.40	1.73
3-fluorophenol	dibutyl ether	1.23	1.00
4-fluorophenol	4-N,N-dimethylaminopyridine	3.15	3.65